

A Two-grid Method for Linearizing and Symmetrizing the Steady-state Poisson-Nernst-Planck Equations

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Abstract

In this paper, a two-grid method is proposed to linearize and symmetrize the steady-state Poisson-Nernst-Planck equations. The computational system is decoupled to linearize and symmetrize equations by using this method, which can improve the computational efficiency compared with the finite element method. Error estimates are derived for the proposed method. The numerical results show that the two-grid method is effective.

Key words. Poisson-Nernst-Planck equations, two-grid method, finite element method, linearization, symmetrization, decoupling

2000 AMS subject classifications. 65N30, 92C40.

1 Introduction

Electrodiffusion model has aroused a well-accepted publicity over the past years due to its widely applications in semiconductors [9, 13, 16], electrochemical systems [2, 14] and biological membrane channels [3, 7, 8]. It is mainly described by the Poisson-Nernst-Planck (PNP) equations, which are a system coupled by the NP equation and the electrostatic Poisson equation. Here the NP equation is nonlinear and nonsymmetric. Due to the nonlinearity and coupling of the PNP equations, in general, it is almost impossible to find the analytic solutions of the equations.

In the past several decades, there appears many literatures on numerical methods for the PNP equations, including finite difference method, finite volume method and finite element method, etc. Finite difference method was widely used to solve the PNP equations [4, 6], but the main disadvantage of it may be the poor adaptability of irregular region. Finite volume method, which focuses on avoiding the disadvantage of finite difference method, was then applied to solve the PNP equations in irregular domains, but it is not easy to achieve the high accuracy owing to the difficulty of the designing higher-order control volume [15, 19]. Finite element method, which is suitable for irregular surface, has shown the efficiency and effectiveness of dealing with the electrodiffusion model [11, 12].

The PNP equations are a kind of coupled system. Generally speaking, it is convenient to solve a coupled system by using a decoupling method than solving it directly. The decoupling method in which the coupled problems can be separated into single subproblems, are interested in applications. The suitable methods are allowed to use flexibly for solving each subproblem separately, and the numerical implementation is easy and efficient. Recently, a decoupling two-grid method for the steady-state PNP equations is proposed in [24]. By using that method, the coupled system is decoupled by the coarse grid finite element approximation and good initial values are provided for solving PNP equations, which can improve the computational efficiency and save the computational time. The theoretical results show that if the finite element solution on the coarse grid approximates that on the fine grid well enough, then

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the two-grid method can achieve the similar approximation effect that the conventional finite element method could do. The numerical results in [24] show the effectiveness of the two-grid method.

Note that the two-grid method, proposed originally by Xu [20] in 1992, is an efficient numerical method for nonselfadjoint or indefinite problems. Later, Xu [21, 22] designed and analyzed the two-grid method for the nonlinear elliptic equations, in which the main idea is to use a solution on the coarse space to produce a rough approximation of the solution, and then use it as the initial guess so that the original equation is linearized on the fine grid. This procedure involves a nonlinear solver on the coarse space and a linear solver on the fine space. Now this idea has been applied to solving many problems, such as nonlinear fourth-order reaction-diffusion problem [10], nonlinear parabolic equations [5] and nonlinear reaction-diffusion equations [18]. In [24], the two-grid method is used to decouple the PNP equations. However, the decoupled system is still a nonlinear system or a linear but asymmetric system, so many excellent algorithms which are suitable for the linear and symmetric system can not be used. In fact, we can apply the idea of two-grid method for the linearization and symmetrization of a single equation to the PNP equations, so a two-grid method for linearizing and symmetrizing the PNP equations is generated.

In this paper, we construct two kinds of two-grid algorithms for linearizing and symmetrizing the PNP equations, which are based on the decoupling two-grid algorithms in [24]. The error estimates are also presented for the algorithms. These error estimates indicate that our two-grid method can retain the same order of approximation accuracy as both the standard finite element method and the two-grid method in [24] do, but our algorithms can be plugged in the most efficient and optimized local linear and symmetric solvers which are more efficient.

The outline of this paper is as follows. Some preliminaries are presented in the next section. Two kinds of two-grid algorithms are proposed and analyzed in section 3. Numerical experiments are demonstrated in section 4.

2 Preliminaries

In this section we aim to describe some notations and briefly review the PNP equations and their variational forms. Besides, we introduce the finite element approximation of the PNP equations and some error bounds of them. Let $\Omega \subset R^d$ ($d = 2, 3$) be a bounded Lipschitz domain. We adopt the standard notations for Sobolev spaces $W^{s,p}(\Omega)$ and their associated norms and seminorms [1]. For $p = 2$, the notations $H^s(\Omega) = W^{s,2}(\Omega)$ and $H_0^1(\Omega) = \{v \in H^1(\Omega) : v|_{\partial\Omega} = 0\}$, where $v|_{\partial\Omega} = 0$ is in the sense of trace, $\|\cdot\|_{s,p,\Omega} = \|\cdot\|_{W^{s,p}(\Omega)}$ are used. Let (\cdot, \cdot) denote the standard L^2 inner product.

We introduce the following steady state PNP equations (see the time-dependent PNP equations in [17])

$$-\nabla \cdot (\nabla p^i + q^i p^i \nabla \phi) = F_i, \quad \text{for } i = 1, 2, \quad (2.1)$$

$$-\Delta \phi = \sum_{i=1}^2 q^i p^i + F_3, \quad (2.2)$$

where $p^i(x) : \Omega \rightarrow R_0^+$ is the concentration of ions, $\phi(x) : \Omega \rightarrow R$ is the electrostatic potential. The index i stands for the different ionic species and q^i is the charge of species i . For simplicity, in the following we choose $q^1 = 1, q^2 = -1$, F_i ($i = 1, 2, 3$) indicate the reaction source terms. In addition, we consider the homogeneous Dirichlet boundary conditions as follows: $p^1 = p^2 = \phi = 0$, on $\partial\Omega$.

The weak formulation of (2.1)-(2.2) reads: find $p^i \in H_0^1(\Omega)$, $i = 1, 2$ and $\phi \in H_0^1(\Omega)$ such that

$$(\nabla p^i, \nabla v) + (q^i p^i \nabla \phi, \nabla v) = (F_i, v), \quad \forall v \in H_0^1(\Omega), \quad i = 1, 2, \quad (2.3)$$

$$(\nabla \phi, \nabla w) = \sum_{i=1}^2 q^i (p^i, w) + (F_3, w), \quad \forall w \in H_0^1(\Omega). \quad (2.4)$$

Let Γ_h be a quasi-uniform triangulation of Ω with mesh size $h > 0$ and define corresponding linear finite element space

$$S_h(\Omega) = \{v \in H^1(\Omega) : v|_{\partial\Omega} = 0 \text{ and } v|_e \in p^1(e), \forall e \in \Gamma_h(\Omega)\}, \quad (2.5)$$

where $p^1(e)$ is the set of linear polynomials. The coarse space $S_H(\Omega)$ is defined by replacing h with H . Moreover, throughout this paper C denotes a positive constant independent of h , but may have different values at different places.

Assume there exists a unique solution (ϕ, p^i) ($i = 1, 2$) satisfying (2.3)-(2.4). The standard finite element approximation of problem (2.3)-(2.4) is defined as flows: find $(p_h^1, p_h^2, \phi_h) \in [S_h(\Omega)]^3$ such that,

$$(\nabla p_h^i, \nabla v_h) + (q^i p_h^i \nabla \phi_h, \nabla v_h) = (F_i, v_h), \quad \forall v_h \in S_h(\Omega), \quad i = 1, 2, \quad (2.6)$$

$$(\nabla \phi_h, \nabla w_h) = \sum_{i=1}^2 q^i(p_h^i, w_h) + (F_3, w_h), \quad \forall w_h \in S_h(\Omega). \quad (2.7)$$

We assume there exists a unique solution (ϕ_h, p_h^i) satisfying (2.6) and (2.7). Some error bounds for the finite element approximations was presented in [23]. If $\phi \in H^{1+m}(\Omega_s)$ and $p^i \in H^{1+m}(\Omega_s)$ ($1 \leq i \leq n, 0 < m \leq 1$), we can obtain

$$\|\phi - \phi_h\|_{1, \Omega_s} \leq C(h^m + \sum_{i=1}^n \|p^i - p_h^i\|_{0, \Omega_s}), \quad (2.8)$$

and

$$\|p^i - p_h^i\|_{1, \Omega_s} \leq C(h^m + \sum_{i=1}^n \|p^i - p_h^i\|_{0, \Omega_s}), \quad (2.9)$$

where $p_h^i \in L^\infty(\Omega_s)$ is assumed.

3 The two-grid algorithms

In this section, two kinds of two-grid algorithms are designed to linearize and symmetrize the PNP equations. Some error estimates are also presented for the algorithms.

We first recall the decoupling two-grid algorithms in [24] which provide a basis for our two-grid algorithms.

Algorithm 3.1. (*the decoupling two-grid Algorithm I [24]*)

Step 1. On the coarse grid, solve the coupled system (2.6) and (2.7) as follows: find $(p_H^1, p_H^2, \phi_H) \in [S_H(\Omega)]^3$, such that

$$(\nabla p_H^i, \nabla v_H) + (q^i p_H^i \nabla \phi_H, \nabla v_H) = (F_i, v_H), \quad \forall v_H \in S_H(\Omega), \quad i = 1, 2, \quad (3.1)$$

$$(\nabla \phi_H, \nabla w_H) = \sum_{i=1}^2 q^i(p_H^i, w_H) + (F_3, w_H), \quad \forall w_H \in S_H(\Omega). \quad (3.2)$$

Step 2. On the fine grid, solve the decoupled system as follows: find $(p_h^{1,}, p_h^{2,*}, \phi_h^*) \in [S_h(\Omega)]^3$, such that*

$$(\nabla p_h^{i,*}, \nabla v_h) + (q^i p_h^{i,*} \nabla \phi_h^*, \nabla v_h) = (F_i, v_h), \quad \forall v_h \in S_h(\Omega), \quad i = 1, 2, \quad (3.3)$$

$$(\nabla \phi_h^*, \nabla w_h) = \sum_{i=1}^2 q^i(p_h^i, w_h) + (F_3, w_h), \quad \forall w_h \in S_h(\Omega). \quad (3.4)$$

Algorithm 3.1 is a semi-decoupling two-grid algorithm, since the solution of density in (3.3) still depends on the solution of potential in (3.4). A fully decoupling algorithm is also presented in [24] as follows:

Algorithm 3.2. (*the decoupling two-grid Algorithm II [24]*)

Step 1. On the coarse grid, solve the coupled system (2.6) and (2.7) as follows: find $(p_H^1, p_H^2, \phi_H) \in [S_H(\Omega)]^3$, such that

$$(\nabla p_H^i, \nabla v_H) + (q^i p_H^i \nabla \phi_H, \nabla v_H) = (F_i, v_H), \quad \forall v_H \in S_H(\Omega), \quad i = 1, 2, \quad (3.5)$$

$$(\nabla \phi_H, \nabla w_H) = \sum_{i=1}^2 q^i (p_H^i, w_H) + (F_3, w_H), \quad \forall w_H \in S_H(\Omega). \quad (3.6)$$

Step 2. On the fine grid, solve the decoupled system as follows: find $(p_h^{1,}, p_h^{2,*}, \phi_h^*) \in [S_h(\Omega)]^3$, such that*

$$(\nabla p_h^{i,*}, \nabla v_h) + (q^i p_h^{i,*} \nabla \phi_H, \nabla v_h) = (F_i, v_h), \quad \forall v_h \in S_h(\Omega), \quad i = 1, 2, \quad (3.7)$$

$$(\nabla \phi_h^*, \nabla w_h) = \sum_{i=1}^2 q^i (p_H^i, w_h) + (F_3, w_h), \quad \forall w_h \in S_h(\Omega), \quad (3.8)$$

Compared with Algorithm 3.1, the system on the fine grid is fully decoupled in this algorithm, so it can be solved in parallel. Note that we have to solve a kind of Nernst-Planck-like equation on the fine grid which is nonlinear asymmetric in Algorithm 3.1 and linear asymmetric in Algorithm 3.2 (see (3.3) and (3.7)). In fact, this kind of equation can be linearized and symmetrized by using the coarse grid solution, which generates the following Algorithm 3.3 and 3.4.

Algorithm 3.3.

Step 1. On the coarse grid, solve the following nonlinear and coupled system for $(p_H^1, p_H^2, \phi_H) \in [S_H(\Omega)]^3$:

$$(\nabla p_H^i, \nabla v_H) + (q^i p_H^i \nabla \phi_H, \nabla v_H) = (F_i, v_H), \quad \forall v_H \in S_H(\Omega), \quad i = 1, 2, \quad (3.9)$$

$$(\nabla \phi_H, \nabla w_H) = \sum_{i=1}^2 q^i (p_H^i, w_H) + (F_3, w_H), \quad \forall w_H \in S_H(\Omega). \quad (3.10)$$

Step 2. On the fine grid, we first solve the Poisson equation for $\phi_h^ \in S_h(\Omega)$:*

$$(\nabla \phi_h^*, \nabla w_h) = \sum_{i=1}^2 q^i (p_H^i, w_h) + (F_3, w_h), \quad \forall w_h \in S_h(\Omega), \quad (3.11)$$

then we solve the following linear and symmetric equation on the fine grid for $(p_h^{1,}, p_h^{2,*}) \in [S_h(\Omega)]^2$:*

$$(\nabla p_h^{i,*}, \nabla v_h) + (q^i p_H^i \nabla \phi_h^*, \nabla v_h) = (F_i, v_h), \quad \forall v_h \in S_h(\Omega), \quad i = 1, 2. \quad (3.12)$$

The Nernst-Planck equation is reduced to a linear and symmetric one on the fine discrete grid by using the coarse grid solution of concentration, which is the difference between Algorithm 3.3 and Algorithm 3.1 (see (3.12) and (3.3)). Since the system on the fine grid is linear symmetric and decoupled, the equations can be solved separately and efficiently by using the existing optimized computing softwares for linear symmetric equations. Next the error analysis for Algorithm 3.3 is presented.

Theorem 3.1. *Let (p_h^i, ϕ_h) , (p_H^i, ϕ_H) and $(p_h^{i,*}, \phi_h^*)$ be the solutions of (2.6)-(2.7), (3.9)-(3.10) and (3.11)-(3.12) respectively, then there holds*

$$\| \nabla(\phi_h - \phi_h^*) \|_{0,\Omega} \leq C \sum_{i=1}^2 \| p_h^i - p_H^i \|_{0,\Omega}. \quad (3.13)$$

Proof. Comparing (2.7) with (3.11), we have

$$(\nabla(\phi_h - \phi_h^*), \nabla w_h) = \sum_{i=1}^2 q^i(p_h^i - p_H^i, w_h), \quad \forall w_h \in S_h(\Omega).$$

Let $w_h = \phi_h - \phi_h^*$ and by Poincaré inequality, we can obtain

$$\begin{aligned} \|\nabla(\phi_h - \phi_h^*)\|_{0,\Omega}^2 &= \left| \sum_{i=1}^2 q^i(p_h^i - p_H^i, \phi_h - \phi_h^*) \right| \\ &\leq C \sum_{i=1}^2 \|p_h^i - p_H^i\|_{0,\Omega} \|\phi_h - \phi_h^*\|_{0,\Omega} \\ &\leq C \sum_{i=1}^2 \|p_h^i - p_H^i\|_{0,\Omega} \|\nabla(\phi_h - \phi_h^*)\|_{0,\Omega}. \end{aligned}$$

Hence, we get

$$\|\nabla(\phi_h - \phi_h^*)\|_{0,\Omega} \leq C \sum_{i=1}^2 \|p_h^i - p_H^i\|_{0,\Omega}.$$

This completes the proof. \square

Theorem 3.2. Let (p_h^i, ϕ_h) , (p_H^i, ϕ_H) and $(p_h^{i,*}, \phi_h^*)$ be the solutions of (2.6)-(2.7), (3.9)-(3.10) and (3.11)-(3.12) respectively, and suppose $\phi_h \in W^{1,\infty}(\Omega)$ and $p_H^i \in L^\infty(\Omega)$, then we have

$$\|\nabla(p_h^i - p_h^{i,*})\|_{0,\Omega} \leq C \sum_{i=1}^2 \|p_h^i - p_H^i\|_{0,\Omega}. \quad (3.14)$$

Proof. Subtracting (2.6) from (3.12), we obtain

$$(\nabla(p_h^i - p_h^{i,*}), \nabla v_h) + (q^i p_h^i \nabla \phi_h - q^i p_H^i \nabla \phi_h^*, \nabla v_h) = 0, \quad \forall v_h \in S_h(\Omega).$$

Setting $v_h = p_h^i - p_h^{i,*}$, we get

$$\begin{aligned} \|\nabla(p_h^i - p_h^{i,*})\|_{0,\Omega}^2 &= |(q^i p_h^i \nabla \phi_h - q^i p_H^i \nabla \phi_h^*, \nabla(p_h^i - p_h^{i,*}))| \\ &\leq C \|p_h^i \nabla \phi_h - p_H^i \nabla \phi_h^*\|_{0,\Omega} \|\nabla(p_h^i - p_h^{i,*})\|_{0,\Omega}. \end{aligned} \quad (3.15)$$

If $\phi_h \in W^{1,\infty}(\Omega)$ and $p_H^i \in L^\infty(\Omega)$, we have

$$\begin{aligned} \|p_h^i \nabla \phi_h - p_H^i \nabla \phi_h^*\|_{0,\Omega} &\leq \|p_h^i \nabla \phi_h - p_H^i \nabla \phi_h\|_{0,\Omega} + \|p_H^i \nabla \phi_h - p_H^i \nabla \phi_h^*\|_{0,\Omega} \\ &\leq \|p_h^i - p_H^i\|_{0,\Omega} + \|\nabla(\phi_h - \phi_h^*)\|_{0,\Omega} \\ &\leq C \sum_{i=1}^2 \|p_h^i - p_H^i\|_{0,\Omega}, \end{aligned} \quad (3.16)$$

where we have used Theorem 3.1. Inserting (3.16) into (3.15), we can easily get the result of Theorem 3.2. This completes the proof. \square

Remark 3.1. Theorem 3.1 and Theorem 3.2 indicate that the H^1 norm errors between the finite element solutions and the solutions in Algorithm 3.3 are governed by the errors between the concentration on the coarse grid (p_H^i) and the concentration on the fine grid (p_h^i) . If we assume p_h^i approximates to p_H^i well enough, for instance,

$$\sum_{i=1}^2 \|p_h^i - p_H^i\|_{0,\Omega} = O(H^2),$$

then we can conclude that the Algorithm 3.3 can retain the same order of approximation accuracy as the standard finite element method does under the condition $h = H^2$, that is

$$\| \nabla(\phi_h - \phi_h^*) \|_{0,\Omega} = O(H^2) = O(h) \quad (3.17)$$

and

$$\| \nabla(p_h^i - p_h^{i,*}) \|_{0,\Omega} = O(H^2) = O(h). \quad (3.18)$$

We will demonstrate the second algorithm as follows.

Algorithm 3.4.

Step 1. On the coarse grid, solve the following nonlinear and coupled system for $(p_H^1, p_H^2, \phi_H) \in [S_H(\Omega)]^3$:

$$(\nabla p_H^i, \nabla v_H) + (q^i p_H^i \nabla \phi_H, \nabla v_H) = (F_i, v_H), \quad \forall v_H \in S_H(\Omega), \quad i = 1, 2, \quad (3.19)$$

$$(\nabla \phi_H, \nabla w_H) = \sum_{i=1}^2 q^i (p_H^i, w_H) + (F_3, w_H), \quad \forall w_H \in S_H(\Omega). \quad (3.20)$$

Step 2. On the fine grid, solve the following linear, symmetric and decoupled system for $(p_h^{1,}, p_h^{2,*}, \phi_h^*) \in [S_h(\Omega)]^3$:*

$$(\nabla p_h^{i,*}, \nabla v_h) = (F_i, v_h) - (q^i p_H^i \nabla \phi_H, \nabla v_h), \quad \forall v_h \in S_h(\Omega), \quad i = 1, 2, \quad (3.21)$$

$$(\nabla \phi_h^*, \nabla w_h) = \sum_{i=1}^2 q^i (p_H^i, w_h) + (F_3, w_h), \quad \forall w_h \in S_h(\Omega). \quad (3.22)$$

In this algorithm, the system in Step 2 is a fully-decoupled one which is the difference between Algorithm 3.3 and Algorithm 3.4. We can treat these two small linear problem (4.5) and (3.22) in parallel which can save a large amount of CPU running time. The difference between Algorithm 3.4 and Algorithm 3.2 is that the system on the fine grid is a symmetric one for the former but an asymmetric one for the latter.

We can get the following error estimates for the solutions of the above algorithm.

Theorem 3.3. *If (p_h^i, ϕ_h) , (p_H^i, ϕ_H) and $(p_h^{i,*}, \phi_h^*)$ are the solutions of (2.6)-(2.7), (3.19)-(3.20) and (4.5)-(3.22) respectively, then we have*

$$\| \nabla(\phi_h - \phi_h^*) \|_{0,\Omega} \leq C \sum_{i=1}^2 \| p_h^i - p_H^i \|_{0,\Omega}. \quad (3.23)$$

The proof of this theorem is the same as Theorem 3.1, since the only difference between Algorithm 3.3 and Algorithm 3.4 is (4.5) which is not used in this proof.

Theorem 3.4. *If (p_h^i, ϕ_h) , (p_H^i, ϕ_H) and $(p_h^{i,*}, \phi_h^*)$ are the solutions of (2.6)-(2.7), (3.19)-(3.20) and (4.5)-(3.22) respectively, $\phi_h \in W^{1,\infty}(\Omega)$ and $p_H^i \in L^\infty(\Omega)$, then we have*

$$\| \nabla(p_h^i - p_h^{i,*}) \|_{0,\Omega} \leq C(\| p_h^i - p_H^i \|_{0,\Omega} + \| \nabla(\phi_h - \phi_H) \|_{0,\Omega}). \quad (3.24)$$

Proof. To derive error estimates, we subtract the equation (2.6) from (4.5), we obtain

$$(\nabla(p_h^i - p_h^{i,*}), \nabla v_h) + (q^i p_h^i \nabla \phi_h - q^i p_H^i \nabla \phi_H, \nabla v_h) = 0, \quad \forall v_h \in S_h(\Omega).$$

Similarly, taking $v_h = p_h^i - p_h^{i,*}$, then

$$\begin{aligned} \| \nabla(p_h^i - p_h^{i,*}) \|_{0,\Omega}^2 &= |(q^i p_h^i \nabla \phi_h - q^i p_H^i \nabla \phi_H, \nabla(p_h^i - p_h^{i,*}))| \\ &\leq C \| p_h^i \nabla \phi_h - p_H^i \nabla \phi_H \|_{0,\Omega} \| \nabla(p_h^i - p_h^{i,*}) \|_{0,\Omega}. \end{aligned} \quad (3.25)$$

Here

$$\begin{aligned} \|p_h^i \nabla \phi_h - p_H^i \nabla \phi_H\|_{0,\Omega} &\leq \|p_h^i \nabla \phi_h - p_H^i \nabla \phi_h\|_{0,\Omega} + \|p_H^i \nabla \phi_h - p_H^i \nabla \phi_H\|_{0,\Omega} \\ &\leq C(\|p_h^i - p_H^i\|_{0,\Omega} + \|\nabla(\phi_h - \phi_H)\|_{0,\Omega}), \end{aligned} \quad (3.26)$$

where the assumptions $\phi_h \in W^{1,\infty}(\Omega)$ and $p_H^i \in L^\infty(\Omega)$ are used. Inserting (3.26) into (3.25), we can easily complete the proof of Theorem 3.4. \square

Remark 3.2. Under the assumption of

$$\sum_{i=1}^2 \|p_h^i - p_H^i\|_{0,\Omega} = O(H^2),$$

we have

$$\|\nabla(\phi_h - \phi_h^*)\|_{0,\Omega} = O(H^2) \quad (3.27)$$

from Theorem 3.3. That means the convergence rate of electrostatic potential in Algorithm 3.4 is consistent with the finite element method if $h = H^2$ is satisfied. Theorem 3.4 suggests that the two-grid solution for the concentration in Algorithm 3.4 has the same accuracy as the finite element solution only when $h = H$, whereas the experiment results in section 4 demonstrate the optimal convergence rate even under the condition of $h \neq H$. This implies the error estimates in Theorem 3.4 may not be the optimal one.

4 Numerical experiment

In this section, we perform a numerical test to show the effectiveness of our algorithms and demonstrate the error estimates we have presented. All the programs are debugged on the Fortran Power Station 4.0 compiler and all results are generated by the same microcomputer.

For simplicity, the domain $\Omega = [0, 1]^3$ is specified and we suppose that the boundary conditions are homogeneous. Furthermore, the right hand side functions are set such that the exact solution (ϕ, p^1, p^2) of (2.1)-(2.2) is as follows

$$\begin{cases} \phi = \sin \pi x \sin \pi y \sin \pi z \\ p^1 = \sin 2\pi x \sin 2\pi y \sin 2\pi z \\ p^2 = \sin 3\pi x \sin 3\pi y \sin 3\pi z. \end{cases}$$

we use piecewise linear finite elements on the tetrahedral mesh to discretize the equations.

To implement Algorithm 3.3, first the Gummel iteration is used on the coarse grid. Given the initial value $(p^{1,0}, p^{2,0}) \in [S_H^0(\Omega)]^2$, for $m \geq 0$ find $(p^{1,m+1}, p^{2,m+1}, \phi^{m+1}) \in [S_H^0(\Omega)]^3$ such that

$$(\nabla \phi^{m+1}, \nabla w) = (F_3, w) + \sum_{i=1}^2 q^i(p^{i,m}, w), \quad \forall w \in S_H^0(\Omega). \quad (4.1)$$

$$(\nabla p^{i,m+1}, \nabla v) + (q^i p^{i,m+1} \nabla \phi^{m+1}, \nabla v) = (F_i, v), \quad \forall v \in S_H^0(\Omega), \quad i = 1, 2. \quad (4.2)$$

The stopping criterion for this iteration is $\|\phi^{m+1} - \phi^m\|_0 < 10^{-5}$. Suppose $p_H^i, i = 1, 2$ is the final solution of the concentration in the above iteration. On the second step, the linear, symmetric and decoupled system is solved by using the coarse grid solution as follows: Find $\phi_h^* \in S_h(\Omega)$, such that

$$(\nabla \phi_h^*, \nabla w_h) = \sum_{i=1}^2 q^i(p_H^i, w_h) + (F_3, w_h), \quad \forall w_h \in S_h(\Omega), \quad (4.3)$$

and find $(p_h^{1,*}, p_h^{2,*}) \in [S_h(\Omega)]^2$:

$$(\nabla p_h^{i,*}, \nabla v_h) + (q^i p_H^i \nabla \phi_h^*, \nabla v_h) = (F_i, v_h), \quad \forall v_h \in S_h(\Omega), \quad i = 1, 2. \quad (4.4)$$

The errors between the exact solutions and two-grid solutions of Algorithm 3.3 are shown in Table 1. The errors in H^1 norm approximate the first-order reduction as $h = H^2$ becomes smaller, which coincides with the theoretical results.

H	h	$\ \phi_h^* - \phi\ _1$	$\ p_h^{1,*} - p^1\ _1$	$\ p_h^{2,*} - p^2\ _1$	CPU(S)
1/2	1/4	9.15E-01	3.03E+00	5.40E+00	0.06
1/4	1/16	2.44E-01	9.79E-01	2.12E+00	1.89
1/8	1/64	6.22E-02	2.58E-01	5.69E-01	503.75

Table 1: The H^1 norm errors between the exact solutions and the two-grid solutions of Algorithm 3.3

The two-grid solutions of Algorithm 3.4 are obtained by using the similar computational procedure in (4.1)-(4.3), but (4.4) is replaced with the following equation:

$$(\nabla p_h^{i,*}, \nabla v_h) = (F_i, v_h) - (q^i p_H^i \nabla \phi_H, \nabla v_h), \quad \forall v_h \in S_h(\Omega), \quad i = 1, 2.$$

The errors between the exact solutions and the two-grid solutions of Algorithm 3.4 are shown in Table 2. The error for the potential ϕ_h^* in H^1 norm approximates the first-order reduction as $h = H^2$ becomes smaller, which coincides with the theoretical result of Theorem 3.3. However, the errors of solutions $p_h^{1,*}$ and $p_h^{2,*}$ can not approximate the first-order reduction respectively under the condition of $h = H^2$, especially when $H = 1/8$ and $h = 1/64$. We consider this phenomenon is due to a low order approximation for $\nabla \phi_H$ to $\nabla \phi_h$ (see Theorem 3.4). This problem can be remedied by using a smaller size of coarse grid (see the result of last row in Table 2).

H	h	$\ \phi_h^* - \phi\ _1$	$\ p_h^{1,*} - p^1\ _1$	$\ p_h^{2,*} - p^2\ _1$	CPU(S)
1/2	1/4	9.15E-01	3.03E+00	5.40E+00	0.04
1/4	1/16	2.44E-01	9.89E-01	2.12E+00	1.81
1/8	1/64	6.22E-02	2.91E-01	5.80E-01	500.06
1/32	1/64	6.09E-02	2.46E-01	5.48E-01	629.04

Table 2: The H^1 norm errors between the exact solutions and the two-grid solutions of Algorithm 3.4

Next, we will compare Algorithm 3.3 and 3.4 with the finite element method. The L^2 norm and H^1 norm errors between the exact solutions and the finite element solutions are shown in Table 3 (cf. [24]). Compared Table 1 with Table 3, we find that the solutions of Algorithm 3.3 remain the same order of accuracy as the finite element solutions but require much less computational time. For the full decoupled Algorithm 3.4, if we choose a suitable coarse mesh size H , we can achieve the similar effect as the finite element method could do by comparing Table 2 with Table 3. In addition, the CPU running time used by Algorithm 3.4 is much less than that of the finite element method, which indicates the effectiveness of Algorithm 3.4. Note that the CPU time can be saved much more if Algorithm 3.4 is implemented on the parallel computers.

Finally, in order to compare the two-grid Algorithms 3.3 and 3.4 with the two-grid Algorithm 3.1 and 3.2 presented in [24], Table 4 and Table 5 list the H^1 norm errors between the exact solutions and the solutions of Algorithm 3.1 and 3.2, respectively, where the numerical results are generated by the same environment as Algorithms 3.3 and 3.4. Both Table 2 and Table 4 show the results of the semi-decoupling algorithms. Table 3 and Table 5 display the results of the full-decoupling algorithms. A comparison of Table 2 with Table 4 shows that there is no big difference in the solutions of Algorithm 3.3 and Algorithm 3.1. However, Algorithm 3.3 is more efficient than Algorithm 3.1 on the CPU running time. Compared Table 3 with Table 5, we can get a similar conclusion for Algorithm 3.4 and 3.2 as the comparison of Algorithm 3.3 with Algorithm 3.1. The improvement of efficiency of Algorithm 3.3 and 3.4 is due to the use of linear and symmetric solver for the system while a nonlinear or an asymmetric solver is used in Algorithm 3.1 and 3.2.

h	$\ p_h^1 - p^1\ _0$	$\ p_h^1 - p^2\ _0$	$\ \phi_h - \phi\ _1$	$\ p_h^1 - p^1\ _1$	$\ p_h^2 - p^2\ _1$	CPU(S)
1/4	2.41E-01	3.26E-01	9.14E-01	3.03E+00	5.39E+00	1.5
1/8	8.99E-02	1.72E-01	4.80E-01	1.82E+00	3.75E+00	—
1/16	2.53E-02	5.59E-02	2.43E-01	9.57E-01	2.10E+00	7.56
1/32	6.51E-03	1.50E-02	1.22E-01	4.85E-01	1.09E+00	—
1/64	1.64E-03	3.83E-03	6.09E-02	2.44E-01	5.47E-01	2991.73

Table 3: The L^2 norm and H^1 norm errors between the exact solutions and the finite element solutions (cf. [24]).

H	h= H^2	$\ \phi_h^* - \phi\ _1$	$\ p_h^{1,*} - p^1\ _1$	$\ p_h^{2,*} - p^2\ _1$	CPU(S)
1/2	1/4	9.15E-01	3.03E+00	5.39E+00	1.2
1/4	1/16	2.44E-01	9.57E-01	2.10E+00	2.2
1/8	1/64	6.22E-02	2.44E-01	5.47E-01	830

Table 4: The H^1 norm errors between the exact solutions and the two-grid solutions of Algorithm 3.1 (cf. [24])

5 Conclusion

In this paper, we construct and analyze a two-grid method for linearizing and symmetrizing the steady-state PNP equations. This method can reduce a nonlinear and coupled system into a linear, symmetric and decoupled system by solving a nonlinear and coupled system on a much smaller space. The numerical results verify the theoretical results and demonstrate the efficiency of the proposed method. Compared to the finite element method and the two-grid method in [24], the new two-grid method can not only save a large amount of CPU running time, but also retain the same order of approximation accuracy as they do. In the future, it is promising to extend this approach to the time-dependent PNP equations and other kinds of modified PNP equations.

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H	h	$\ \phi_h^* - \phi\ _1$	$\ p_h^{1,*} - p^1\ _1$	$\ p_h^{2,*} - p^2\ _1$	CPU(S)
1/2	1/4	9.15E-01	3.03E+00	5.39E+00	1.2
1/4	1/16	2.44E-01	9.89E-01	2.10E+00	2.2
1/8	1/64	6.22E-02	2.92E-01	5.70E-01	830
1/32	1/64	6.09E-02	2.46E-01	5.48E-01	1189

Table 5: The H^1 norm errors between the exact solutions and the two-grid solutions of Algorithm 3.2 (cf. [24])

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